

## Supplementary Materials

### Structural characterization and assessment of the tyrosinase activity of polyphenols from *Melastoma normale*

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Figure S1. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of **1**

Figure S2. <sup>13</sup>C NMR (125 MHz, Methanol-*d*<sub>4</sub>) spectrum of **1**

Figure S3. HSQC spectrum of **1** in Methanol-*d*<sub>4</sub>

Figure S4. HMBC spectrum of **1** in Methanol-*d*<sub>4</sub>

Figure S5. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **1** in Methanol-*d*<sub>4</sub>

Figure S6. Roesy spectrum of **1** in Methanol-*d*<sub>4</sub>

Figure S7. HRESIMS spectrum of **1**

Figure S8. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of **2**

Figure S9. DEPTQ (125 MHz, Methanol-*d*<sub>4</sub>) spectrum of **2**

Figure S10. HSQC spectrum of **2** in Methanol-*d*<sub>4</sub>

Figure S11. HMBC spectrum of **2** in Methanol-*d*<sub>4</sub>

Figure S12. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **2** in Methanol-*d*<sub>4</sub>

Figure S13. HRESIMS spectrum of **2**

Figure S14. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of **3**

Figure S15. DEPTQ (125 MHz, Methanol-*d*<sub>4</sub>) spectrum of **3**

Figure S16. HSQC spectrum of **3** in Methanol-*d*<sub>4</sub>

Figure S17. HMBC spectrum of **3** in Methanol-*d*<sub>4</sub>

Figure S18. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in Methanol-*d*<sub>4</sub>

Figure S19. HRESIMS spectrum of **3**

Figure S20. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of **4**

Figure S21. DEPTQ (125 MHz, Methanol-*d*<sub>4</sub>) spectrum of **4**

Figure S22. HSQC spectrum of **4** in Methanol-*d*<sub>4</sub>

Figure S23. HMBC spectrum of **4** in Methanol-*d*<sub>4</sub>

Figure S24. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **4** in Methanol-*d*<sub>4</sub>

Figure S25. HRESIMS spectrum of **4**

Figure S26. CD spectrum of **1–4**

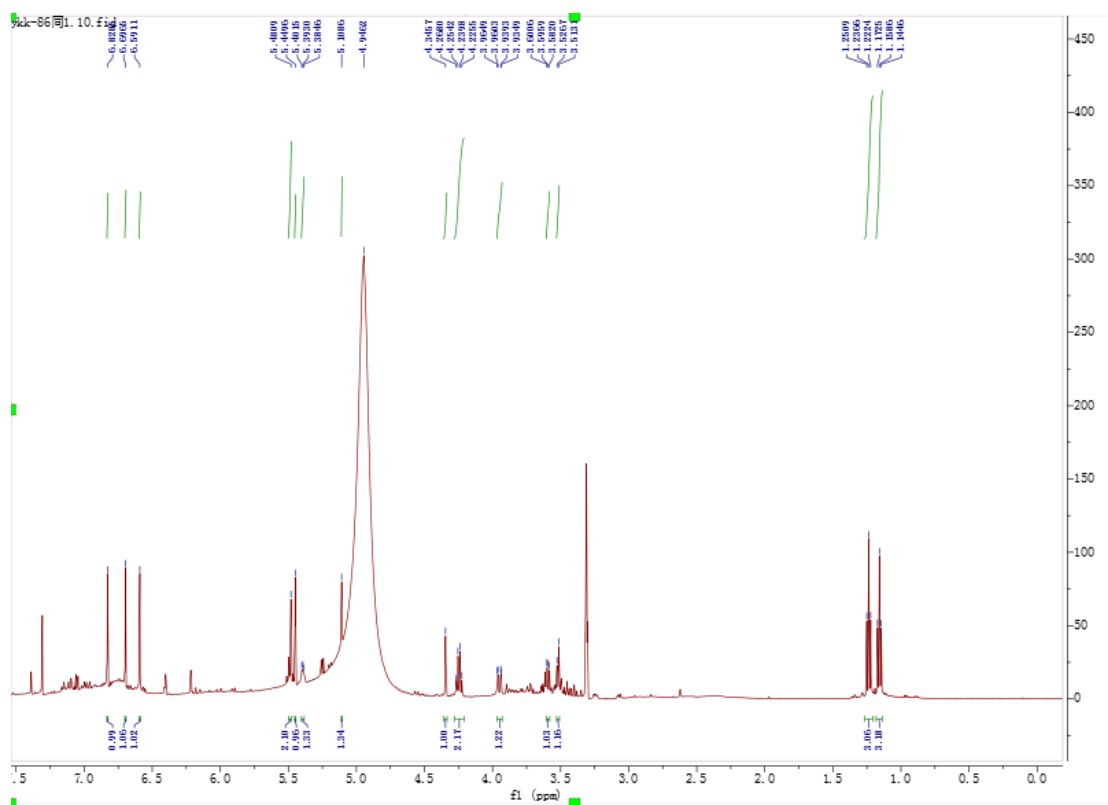


Figure S1. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of 1

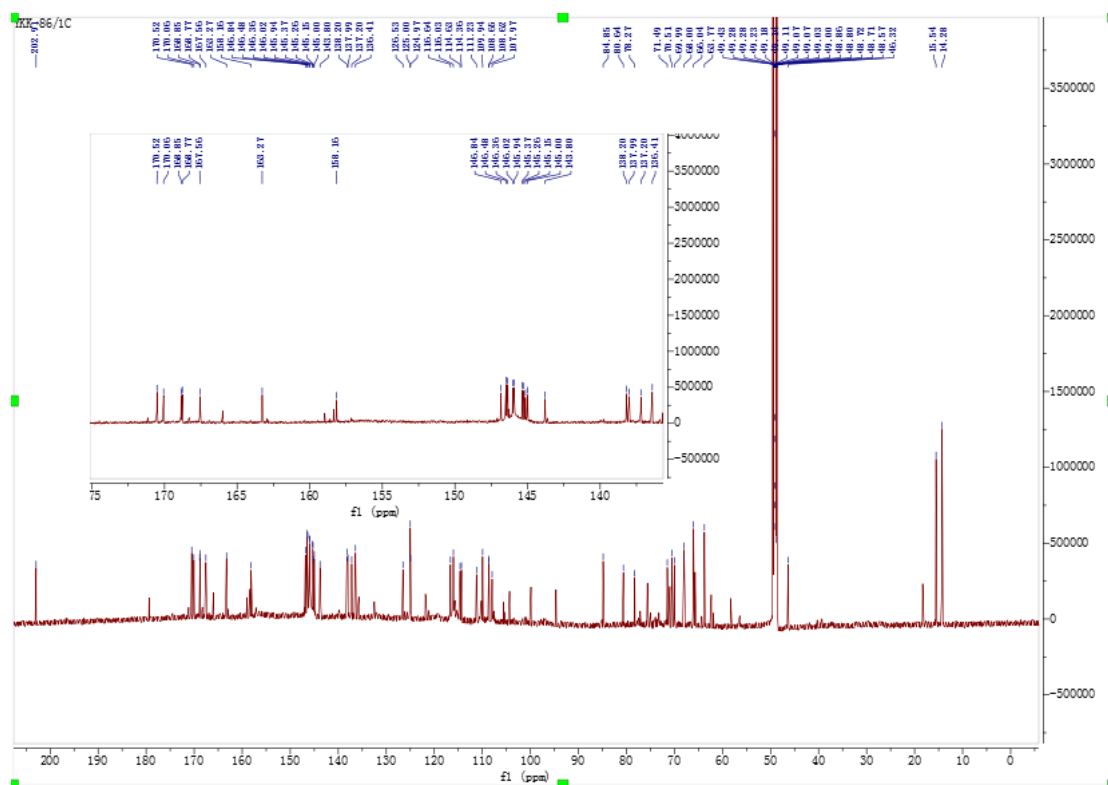


Figure S2. <sup>13</sup>C NMR (125 MHz, Methanol-*d*<sub>4</sub>) spectrum of 1

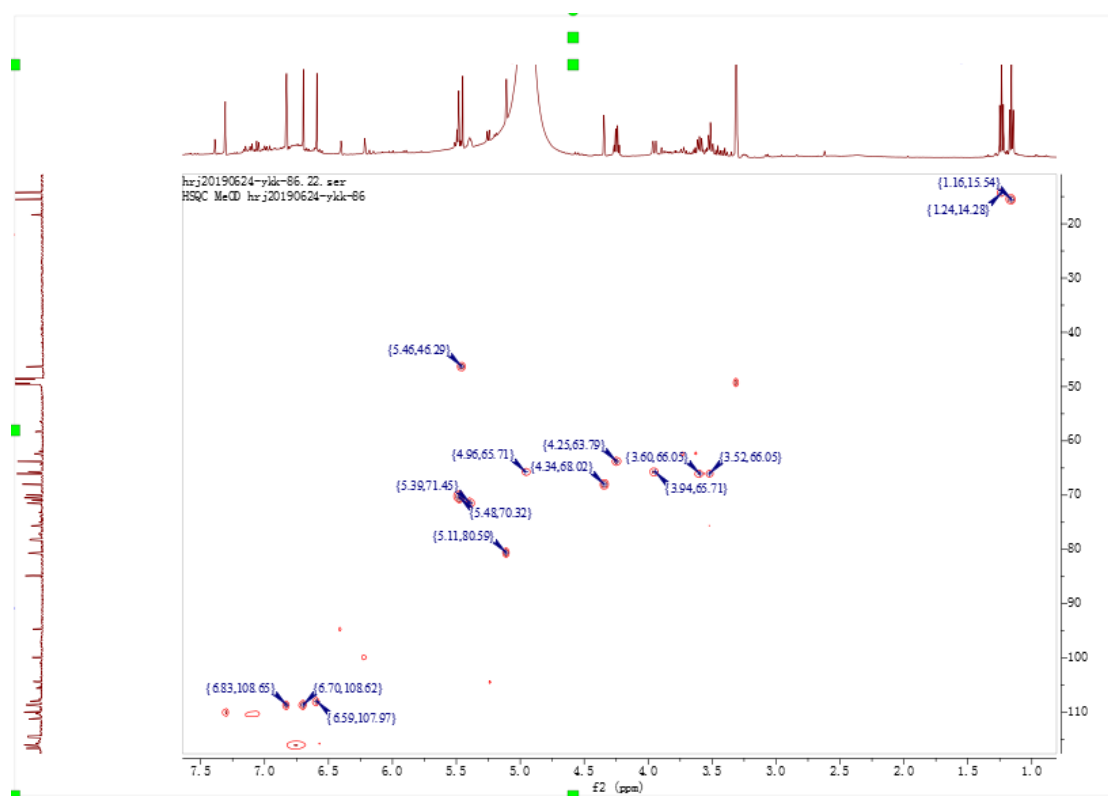


Figure S3. HSQC spectrum of **1** in Methanol- $d_4$

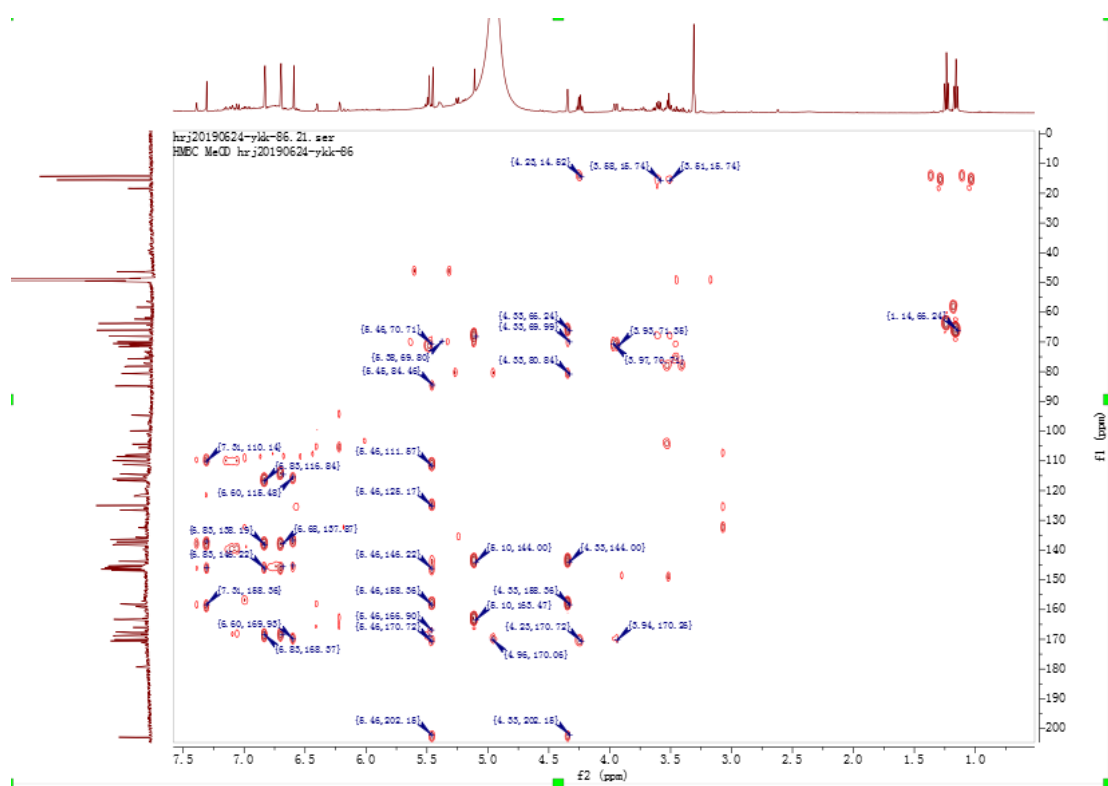


Figure S4. HMBC spectrum of **1** in Methanol- $d_4$

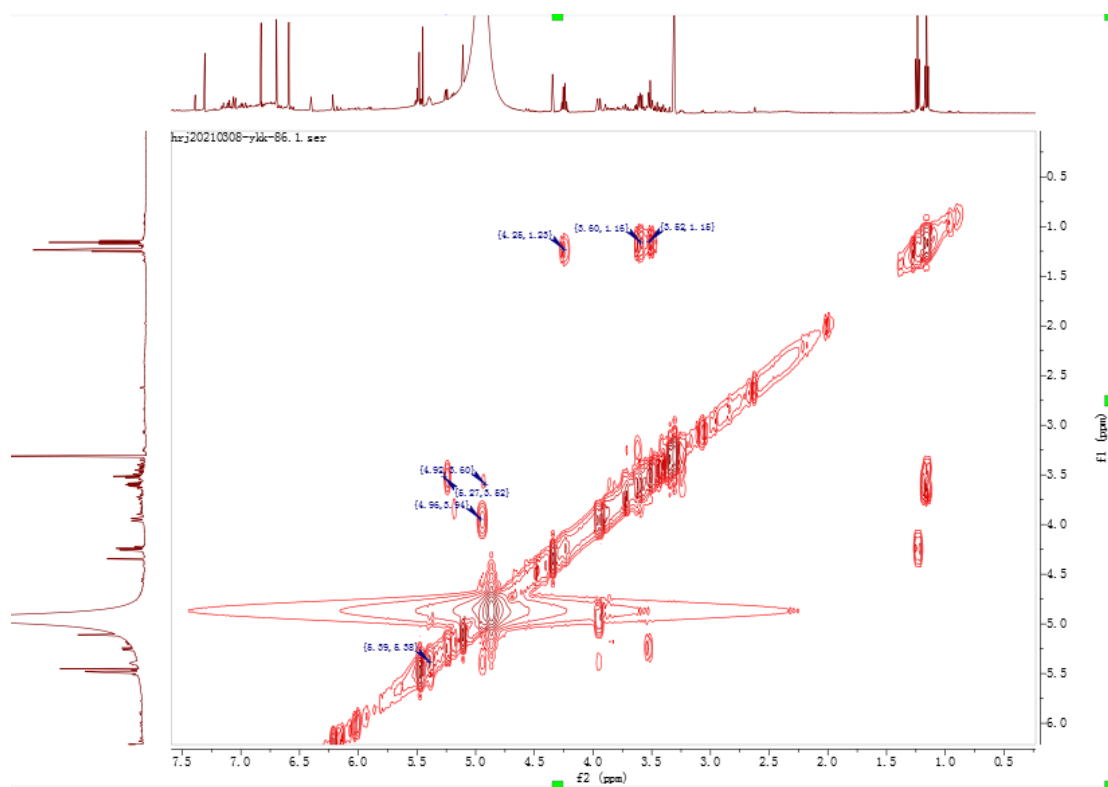


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in Methanol- $d_4$

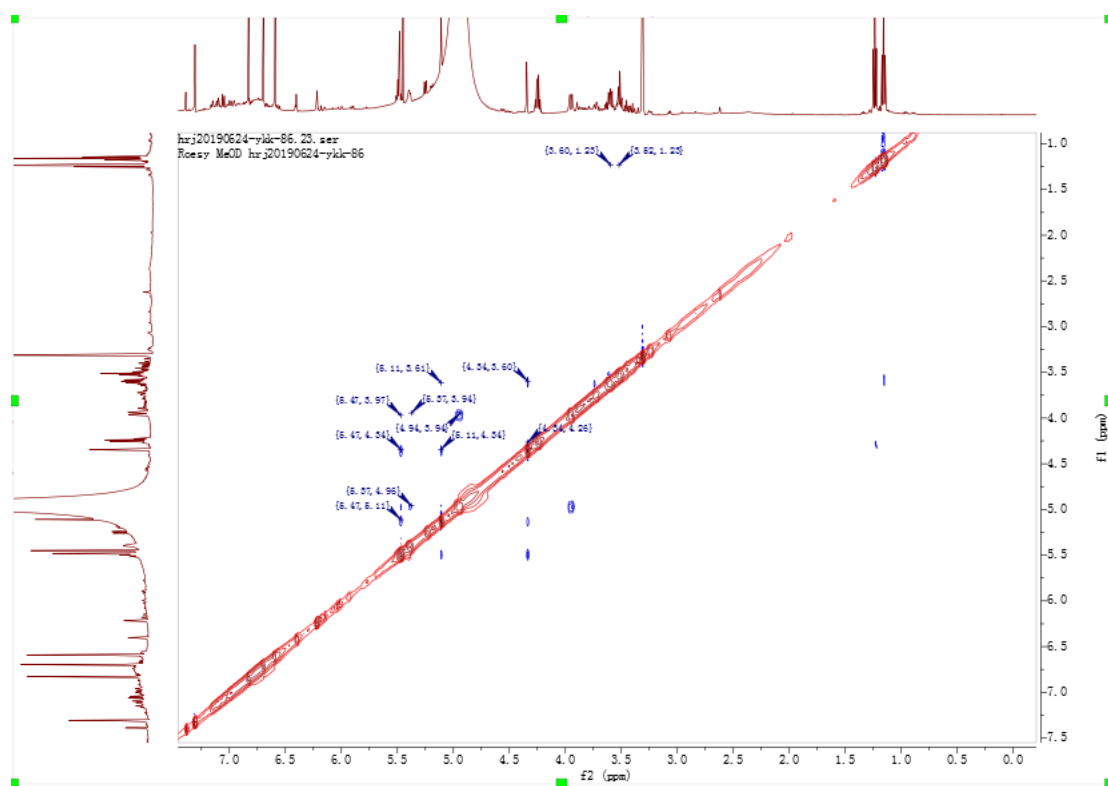


Figure S6. Roesy spectrum of **1** in Methanol- $d_4$

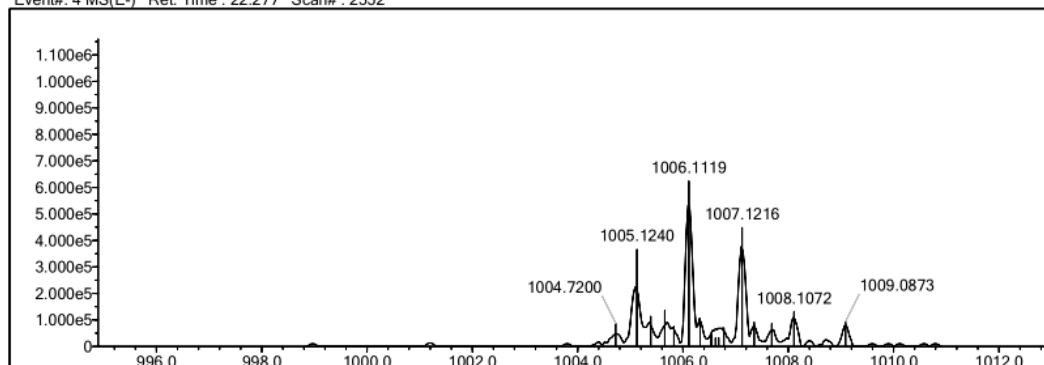
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	1	100	O	2	1	100	H
C	4	1	100	S	2	0	0	
N	3	0	0					

Error Margin (ppm): 50  
 HC Ratio: 0.1 - 4.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: 1.0 - 50.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 500

Event#: 4 MS(E-) Ret. Time : 22.277 Scan#: 2552



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	DBE	Df. (ppm)	Iso	Meas. (M)
2	18.75	C45 H34 O27	[M-H]-	1005.1240	1005.1215	29.0	2.49	19.48	1006.1313

Figure S7. HRESIMS spectrum of 1

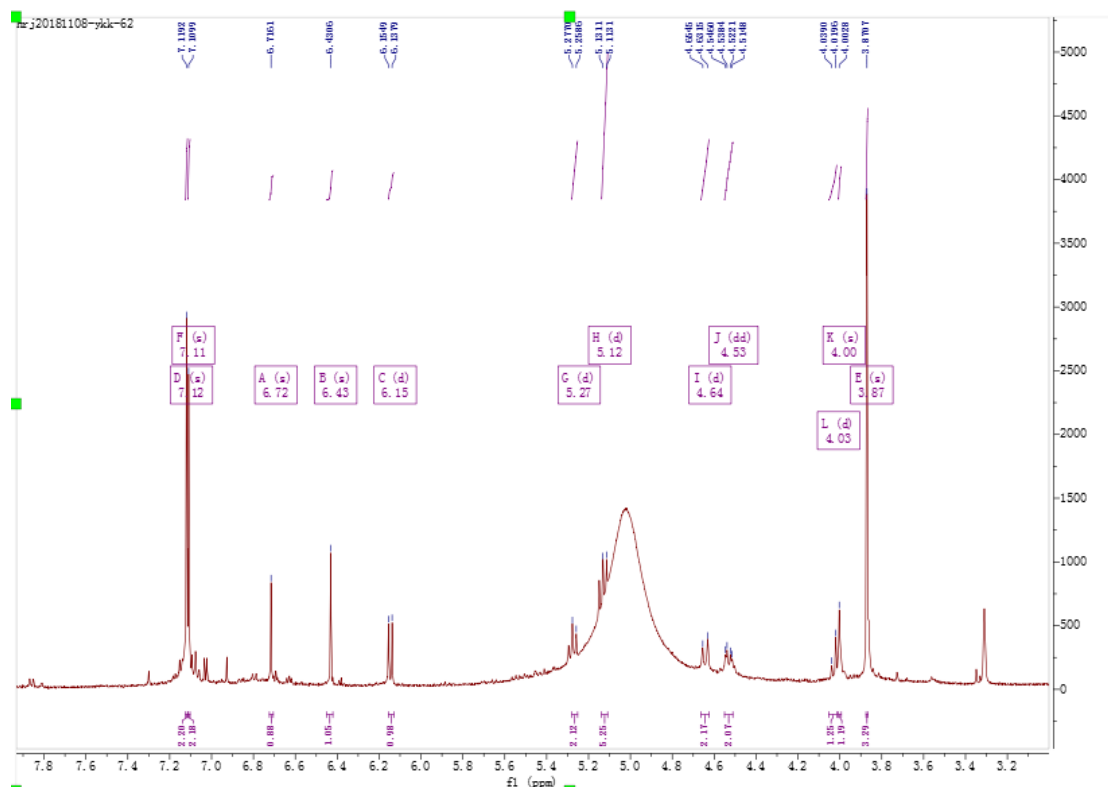


Figure S8. <sup>1</sup>H NMR (500 MHz, Methanol-*d*<sub>4</sub>) spectrum of 2

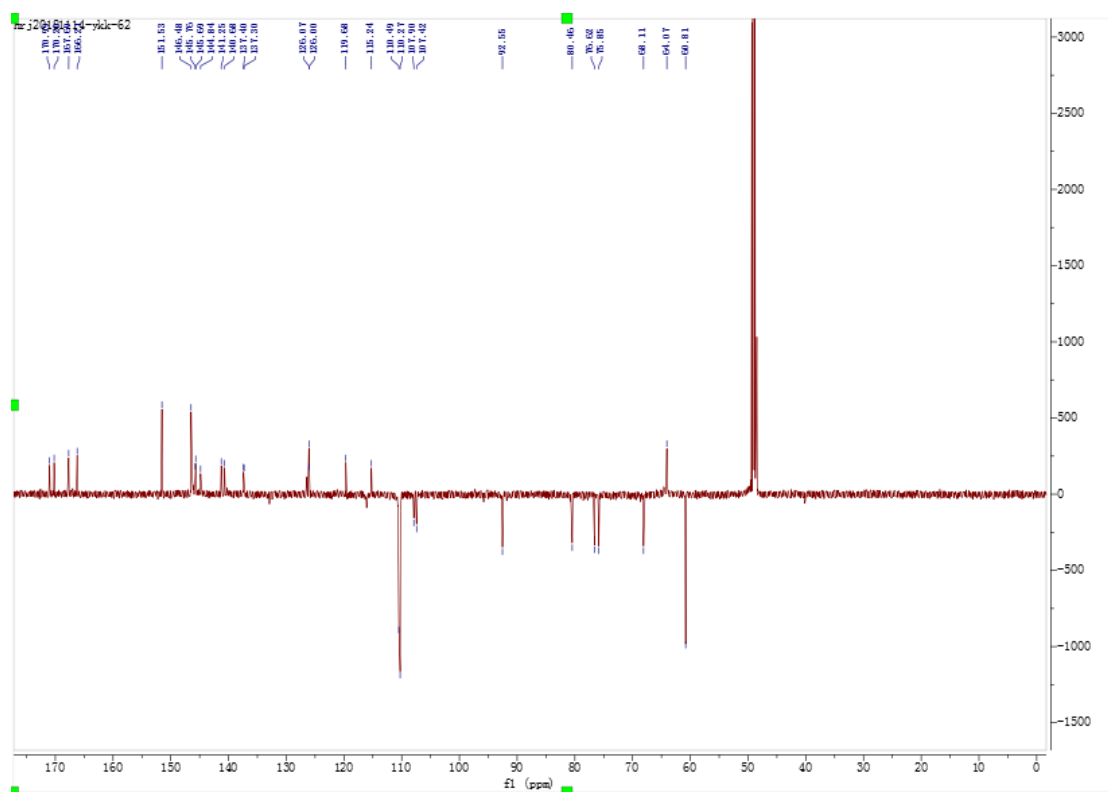


Figure S9. DEPTQ (125 MHz, Methanol- $d_4$ ) spectrum of **2**

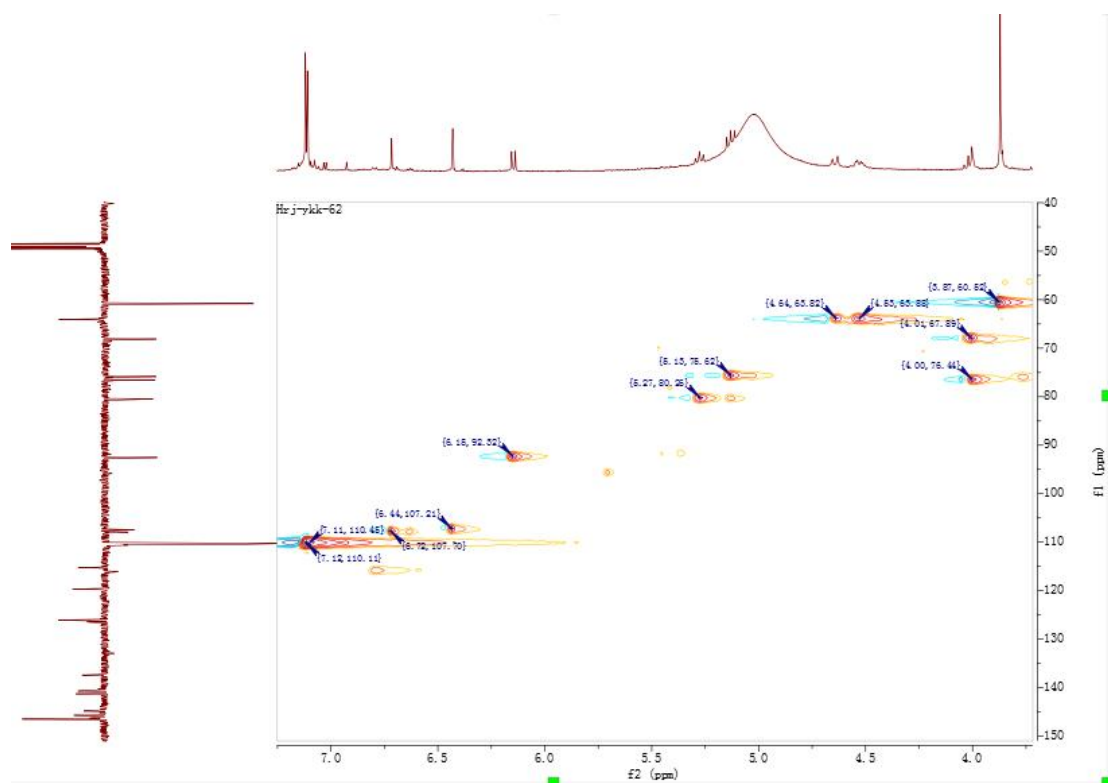


Figure S10. HSQC spectrum of **2** in Methanol- $d_4$

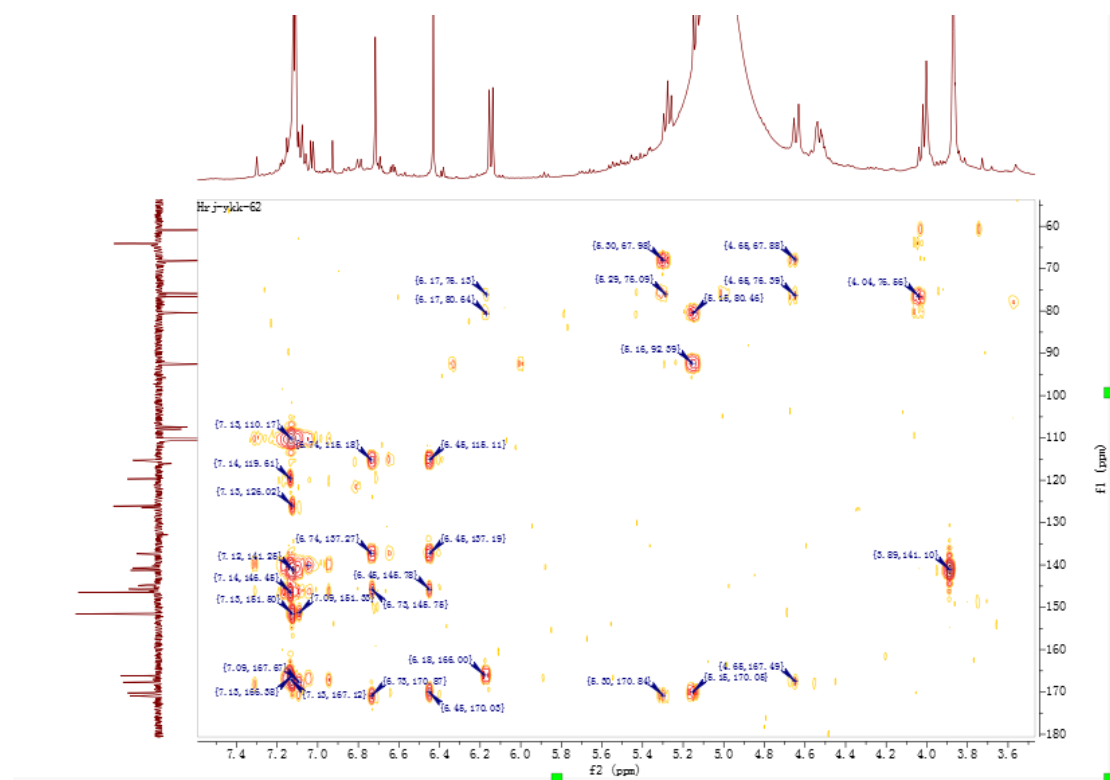


Figure S11. HMBC spectrum of **2** in Methanol-*d*<sub>4</sub>

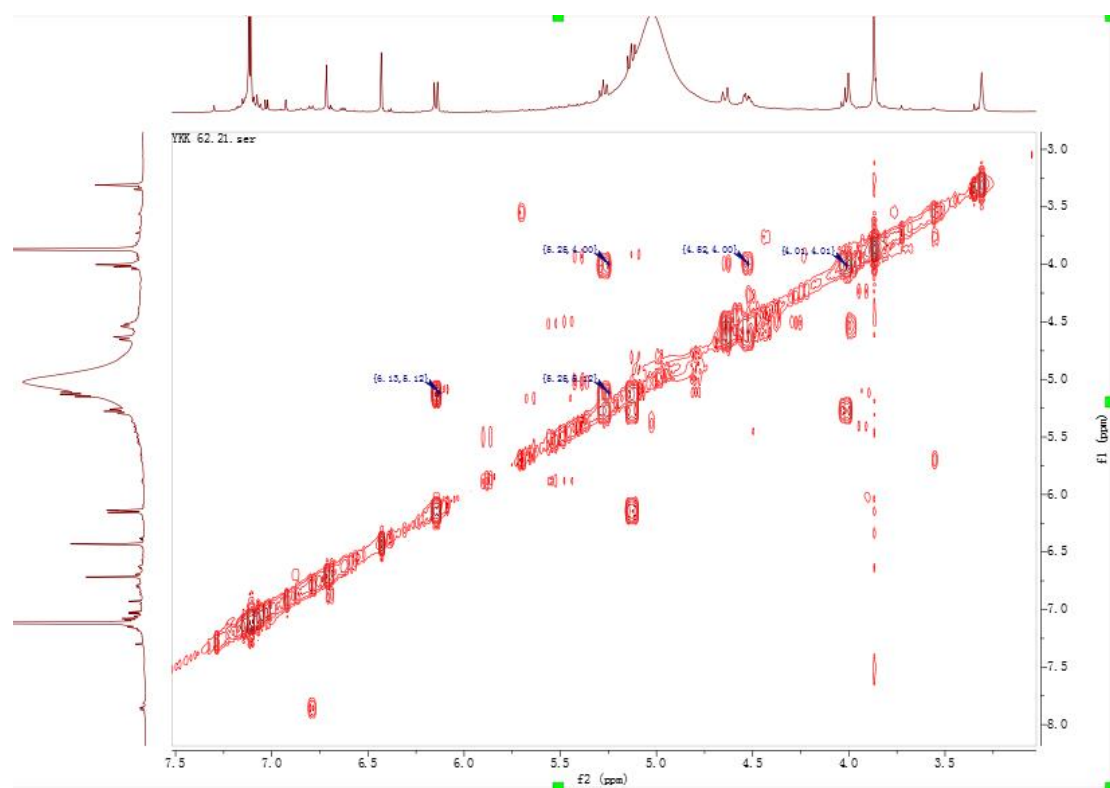
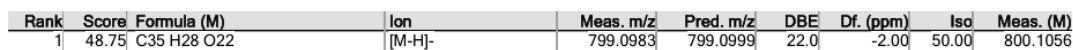


Figure S12. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **2** in Methanol-*d*<sub>4</sub>

Error Margin (ppm): 50	DBE Range: 1.0 - 50.0	Electron Ions: both
HC Ratio: 0.1 - 4.0	Apply N Rule: no	Use MSn Info: no
Max Isotopes: all	Isotope RI (%): 1.00	Isotope Res: 10000
MSn Iso RI (%): 75.00	MSn Logic Mode: AND	Max Results: 500



**1H NMR Spectrum Data:**

Chemical Shift (ppm)	Integration
7.2462	0.95
7.2438	2.00
7.2388	1.00
7.2043	1.00
6.7025	1.05
6.4260	1.17
6.3374	1.29
6.3204	1.29
5.2568	1.35
5.2474	1.26
5.2432	1.05
5.2370	1.11
5.1095	1.05
5.0929	1.11
4.7065	1.05
4.6971	1.26
4.6929	1.05
4.4446	1.05
3.9328	1.05
3.9282	1.11
3.7799	1.05
3.5686	1.11
3.5575	1.05
3.3847	1.05

Figure S14.  $^1\text{H}$  NMR (500 MHz, Methanol- $d_4$ ) spectrum of **3**



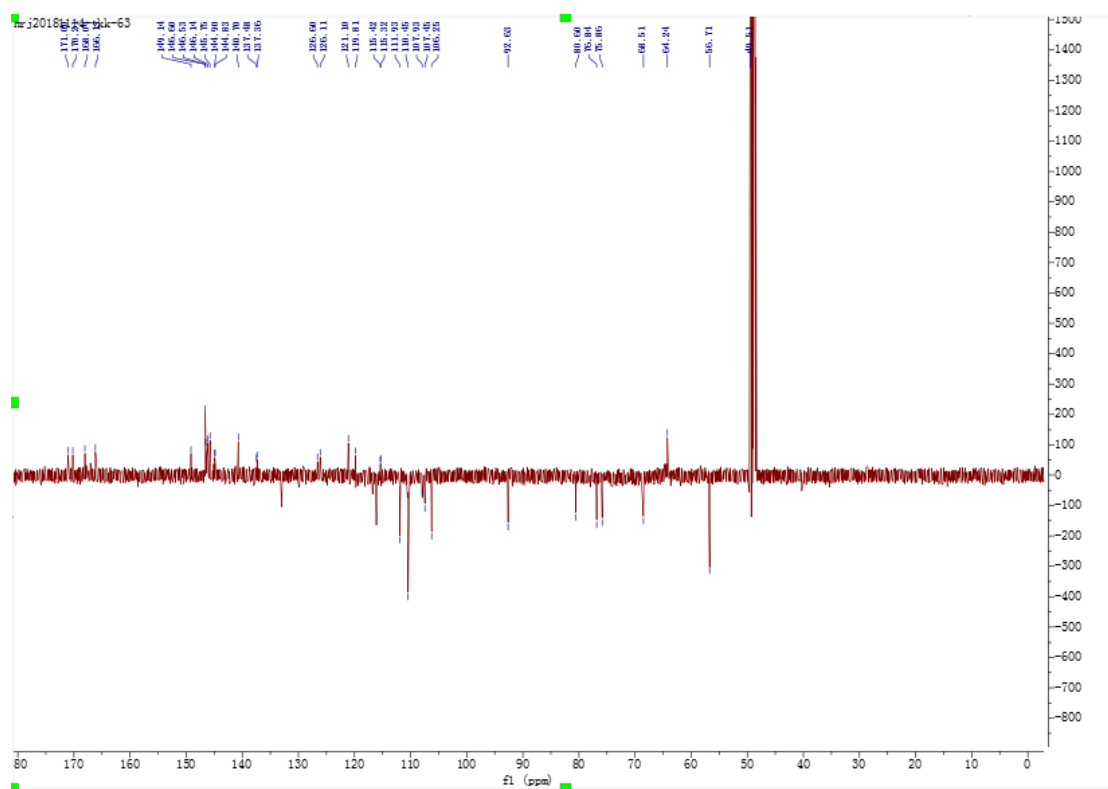


Figure S15. DEPTQ (125 MHz, Methanol- $d_4$ ) spectrum of **3**

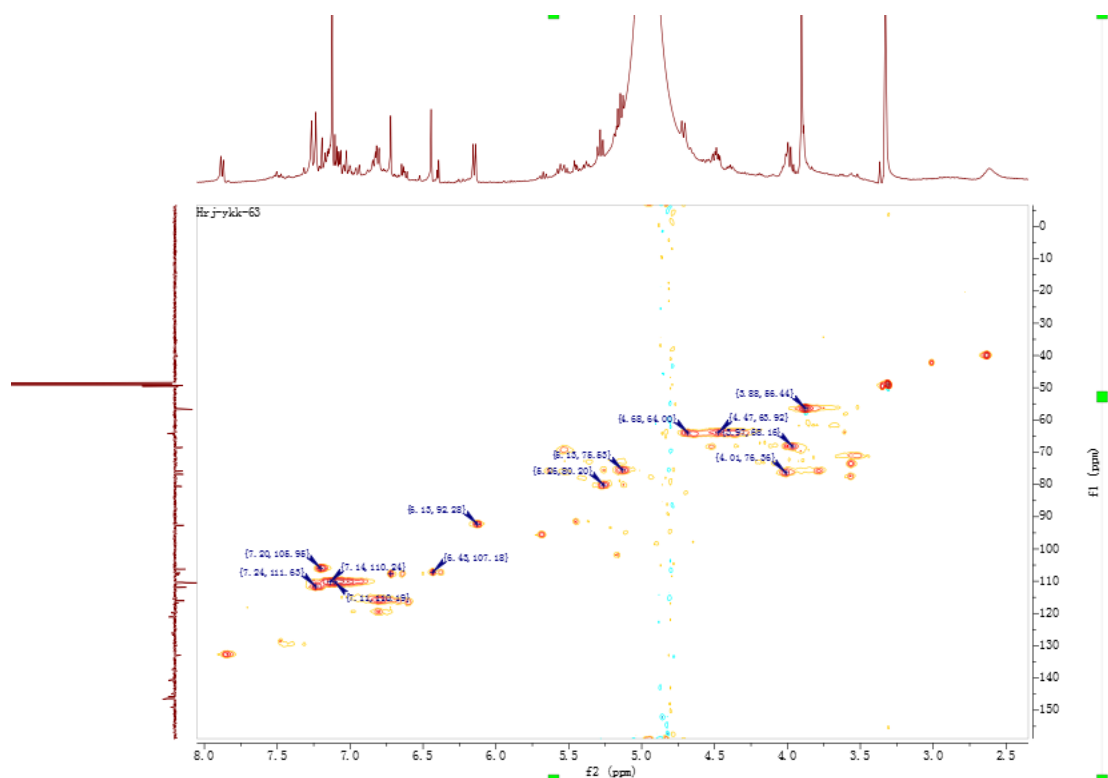


Figure S16. HSQC spectrum of **3** in Methanol- $d_4$

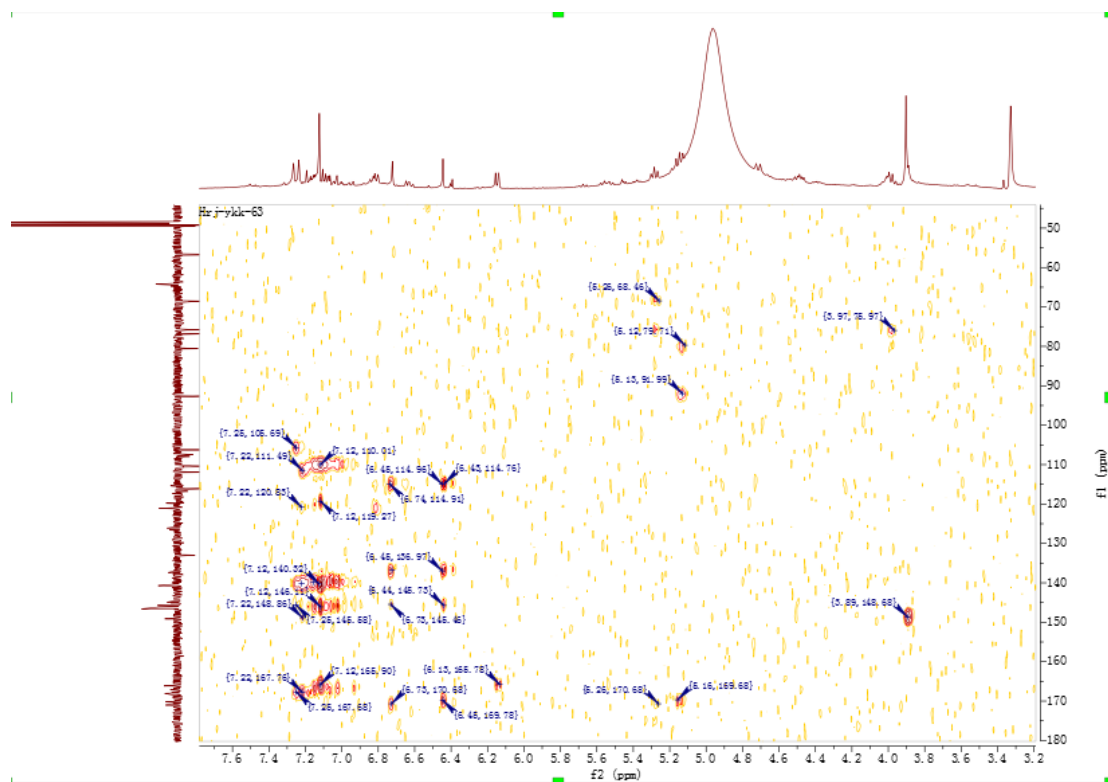


Figure S17. HMBC spectrum of **3** in Methanol-*d*<sub>4</sub>

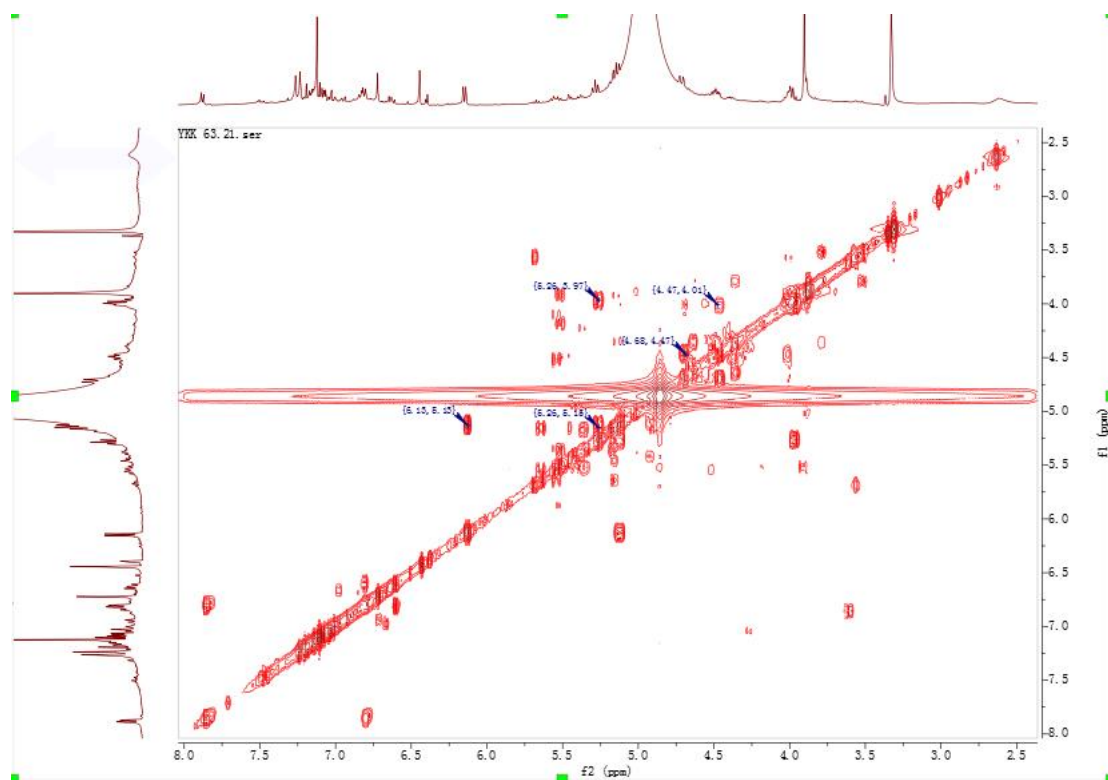


Figure S18. <sup>1</sup>H-<sup>1</sup>H COSY spectrum of **3** in Methanol-*d*<sub>4</sub>

Data File: F:\黄永林&何瑞杰课题组\HRJ-YKK-63.lcd

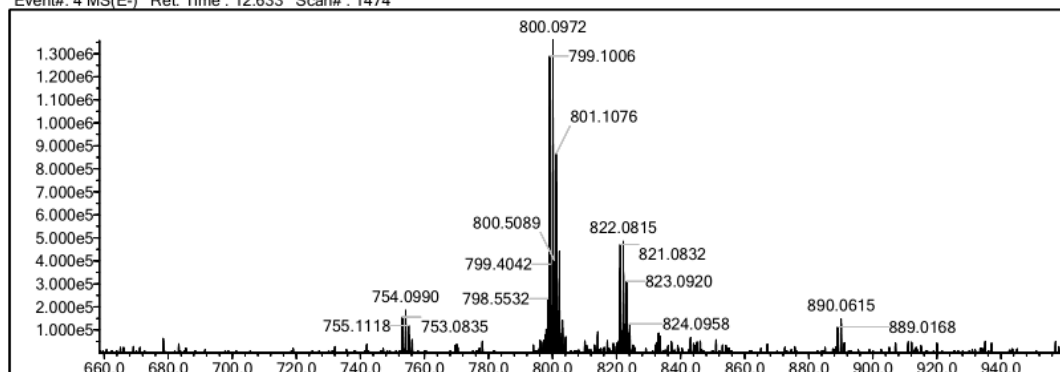
Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	1	100	O	2	1	100	H
C	4	1	100	S	2	0	0	
N	3	0	0					

Error Margin (ppm): 50  
 HC Ratio: 0.1 - 4.0  
 Max Isotopes: all  
 MSn Iso RI (%): 75.00

DBE Range: 1.0 - 50.0  
 Apply N Rule: no  
 Isotope RI (%): 1.00  
 MSn Logic Mode: AND

Electron Ions: both  
 Use MSn Info: no  
 Isotope Res: 10000  
 Max Results: 500

Event#: 4 MS(E-) Ret. Time : 12.633 Scan#: 1474



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	DBE	Df. (ppm)	Iso	Meas. (M)
1	46.30	C35 H28 O22	[M-H]-	799.1006	799.0999	22.0	0.88	46.30	800.1079

Figure S19. HRESIMS spectrum of **3**

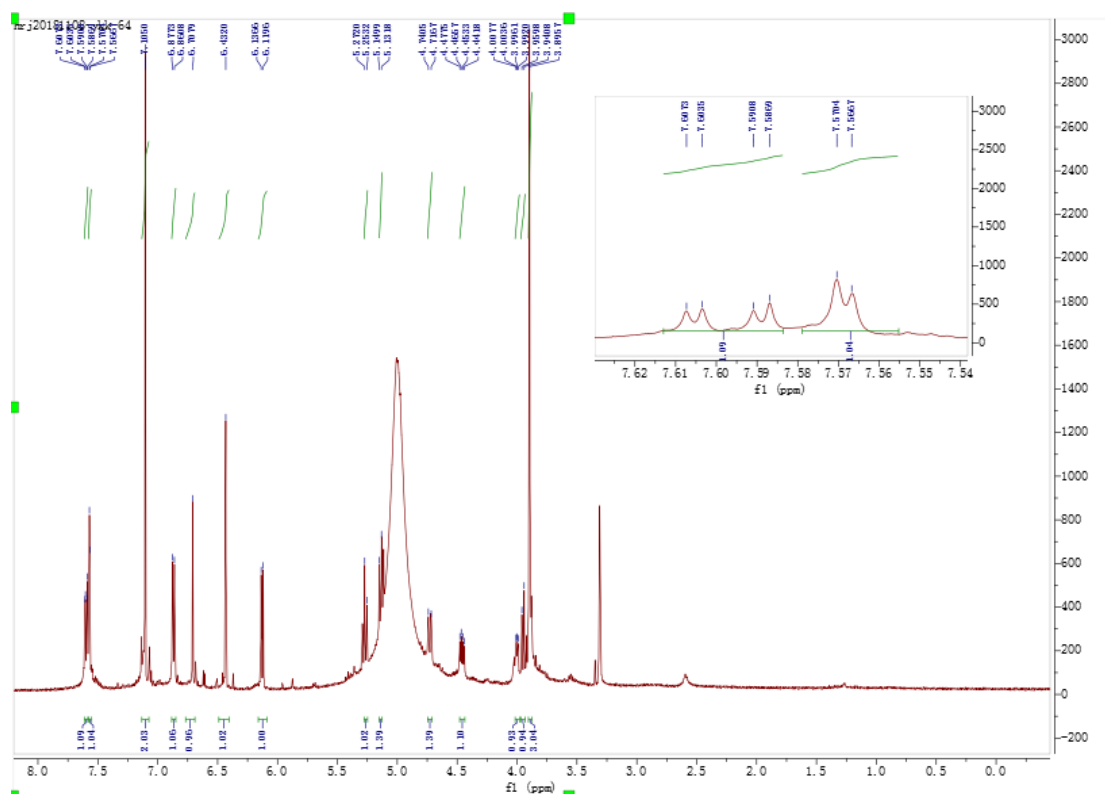


Figure S20.  $^1\text{H}$  NMR (500 MHz, Methanol- $d_4$ ) spectrum of **4**

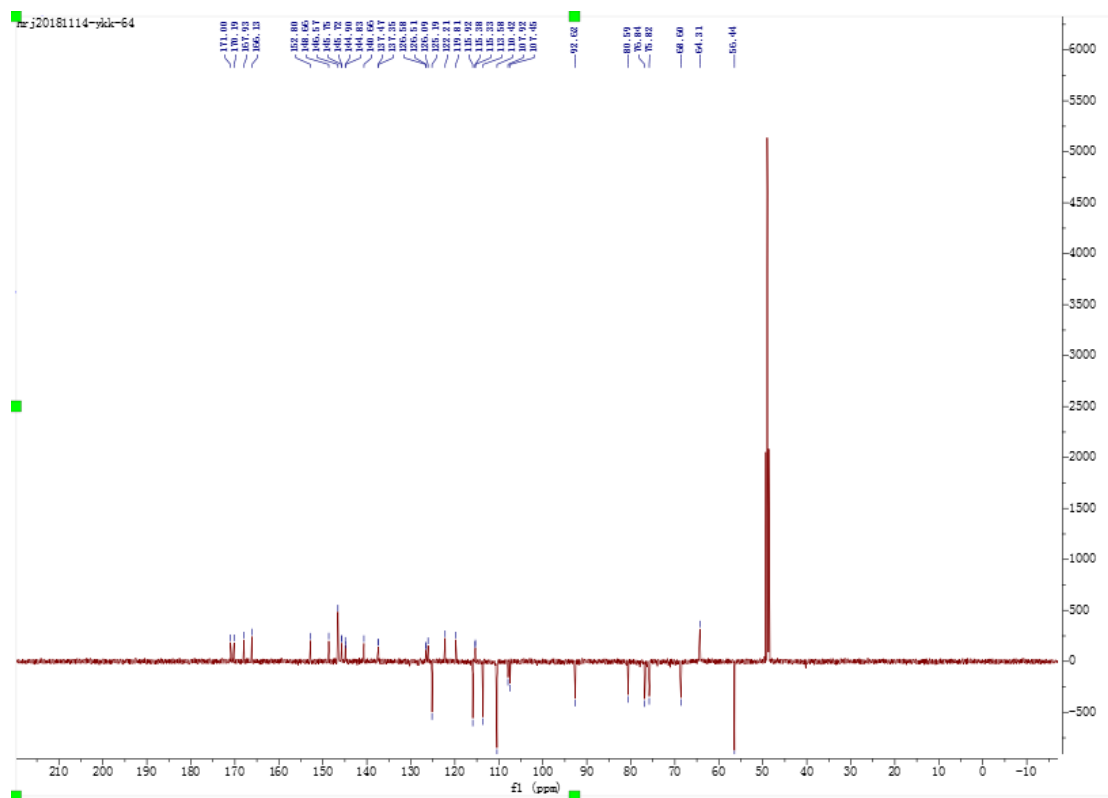


Figure S21. DEPTQ (125 MHz, Methanol- $d_4$ ) spectrum of **4**

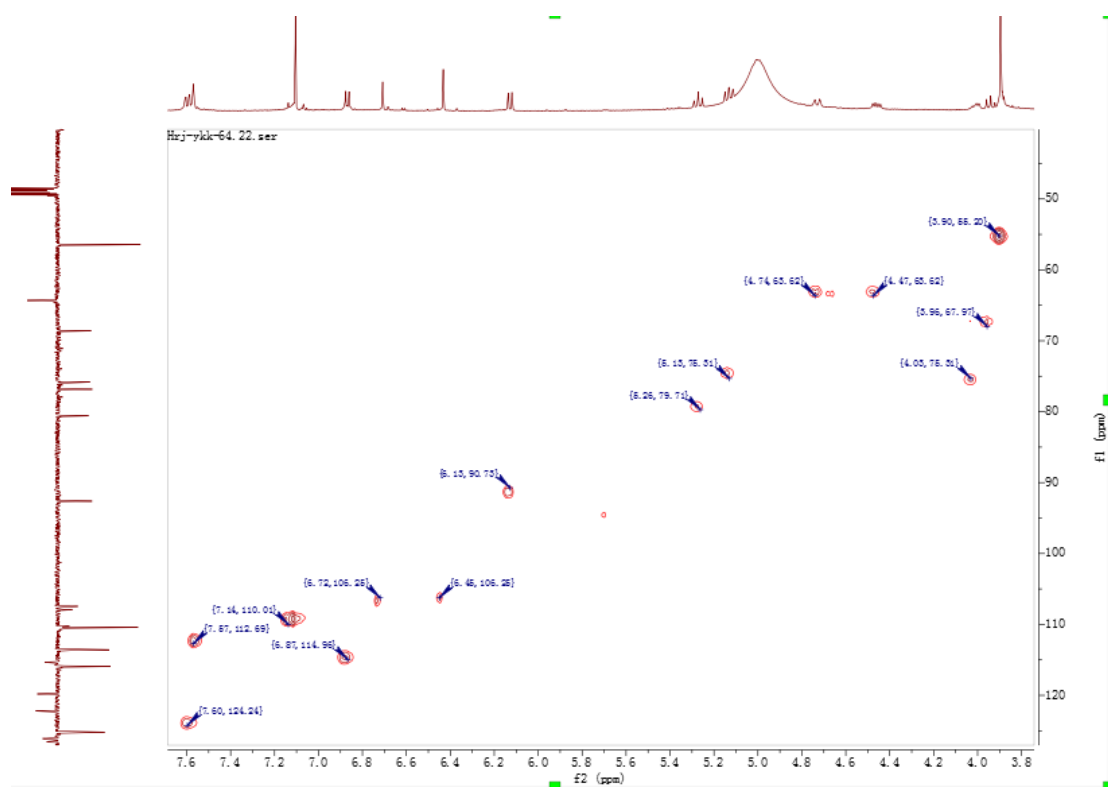


Figure S22. HSQC spectrum of **4** in Methanol- $d_4$

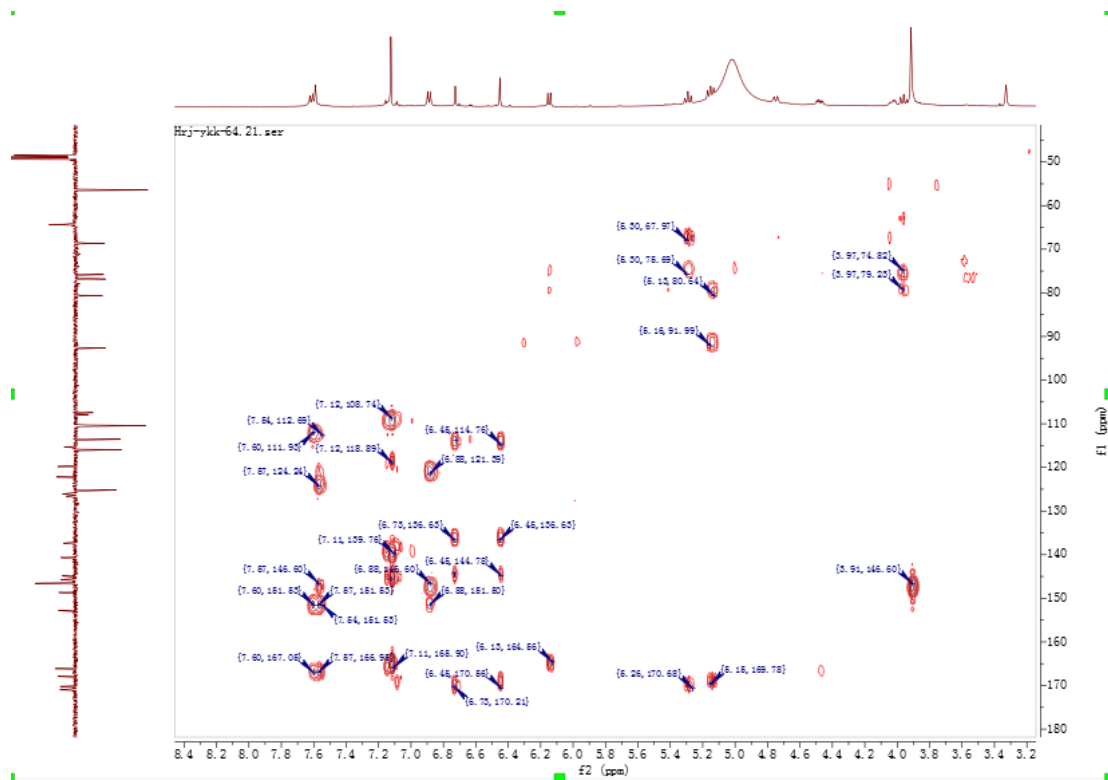


Figure S23. HMBC spectrum of **4** in Methanol- $d_4$

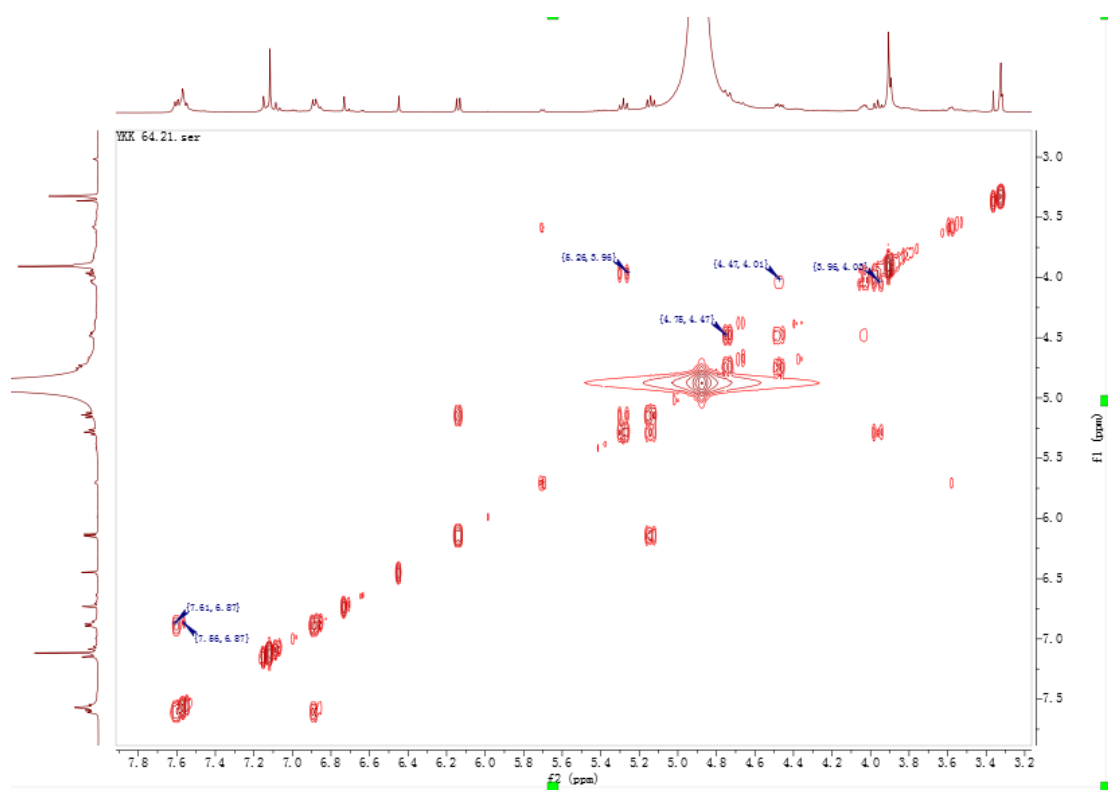


Figure S24.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in Methanol- $d_4$

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	1	100	O	2	1	100	H
C	4	1	100	S	2	0	0	
N	3	0	0					

Error Margin (ppm): 50

HC Ratio: 0.1 - 4.0

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: 1.0 - 50.0

Apply N Rule: no

Isotope RI (%): 1.00

MSn Logic Mode: AND

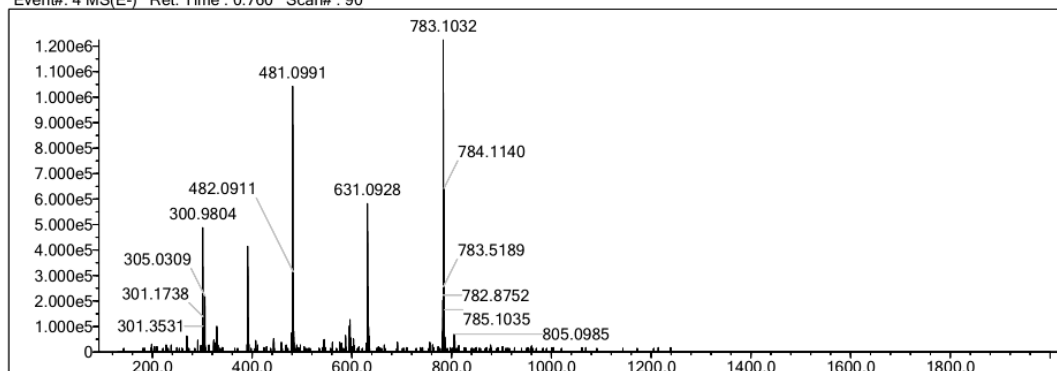
Electron Ions: both

Use MSn Info: no

Isotope Res: 10000

Max Results: 500

Event#: 4 MS(E-) Ret. Time : 0.760 Scan# : 90



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	DBE	Df. (ppm)	Iso	Meas. (M)
2	54.38	C35 H28 O21	[M-H]-	783.1032	783.1050	22.0	-2.30	56.21	784.1105

Figure S25. HRESIMS spectrum of **4**

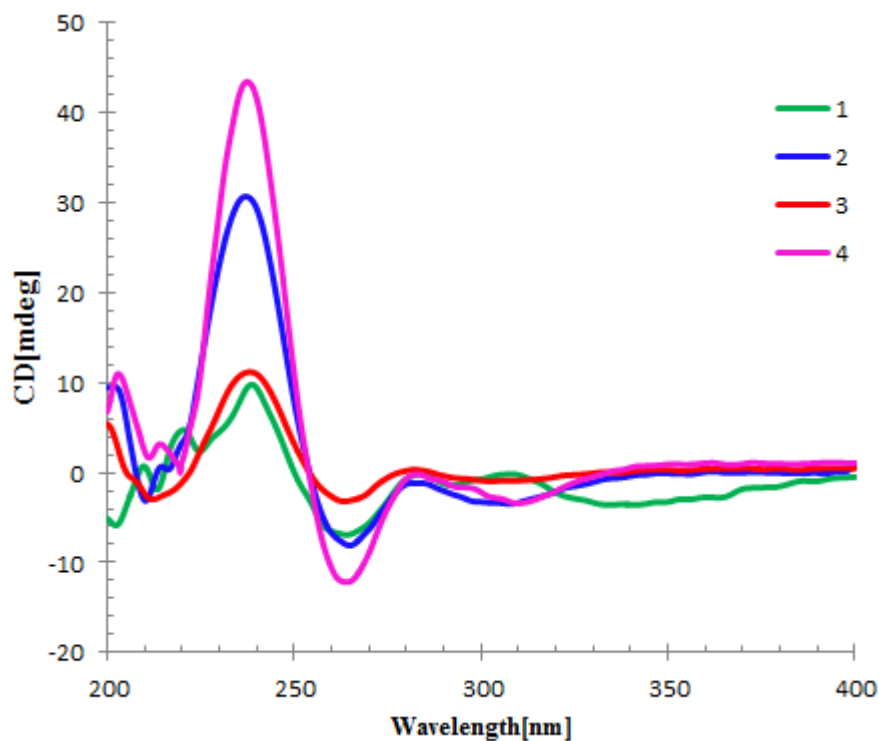


Figure S26. CD spectrum of **1–4**